PROJECT NUMBER: 1752
PROJECT TITLE: Optical Spectroscopy of Tobacco and Smoke
PROJECT LEADER: G. Vilcins
PERIOD COVERED: April, 1989

I. SMOKE CHEMISTRY OF REDUCED DENSITY ROD CIGARETTES

A. **Objective**: To analyze the smoke condensates from low density rod cigarettes.

B. **Results**: The smoke data from the low density rod (LDR) model (X6D9GL) and three controls (X6D9GM, X6D9GN, and X6D9GK) were scaled to a per mg CSC, per puff and per cigarette basis. Factor Analysis in BMDP was used to process the data because of its ability to compare the four cigarettes simultaneously. Different scaling methods yielded the same information. In basic fraction, Factor 1, containing volatile pyridines, pyrazines, quinolines, and quinoxline as the main contributors, separated the cigarettes with and without pectin. The cigarettes with pectin delivered higher amounts of these bases per mg of condensate. The increased delivery of the volatile bases could be due to the citrus pectin providing an additional source of reducing sugars for temperature-induced browning reactions. Factor analysis of the acidic fraction was dominated by one factor. Factor 1 again differentiated the cigarettes by the added citrus pectin. The increased delivery of several simple phenols in the K and L cigarettes probably was due to the breakdown of the added citrus pectin. However, none of these compounds were found to be significantly different. The differentiation of the cigarettes by the neutral fraction also was driven by the pectin factor. The pectin-containing cigarettes delivered more sugar-related degradation products, such as indole, cyclopentanones, furans, and furfural than the non-citrus pectin cigarettes.

C. **Conclusions**: The smoke chemistry in the low density cigarettes mainly is driven by the presence of the additional citrus pectin. By comparing with the controls, the pectin increased the delivery of many volatile bases, simple phenols, and sugar degradation products with the basic compounds being the most influential. The simple phenols and sugar degradation products result directly from the breakdown of pectin while the basic substances probably are due to the browning reaction from the additional reducing sugar source. Even though the added pectin evidently was involved either directly or indirectly in the smoke chemistry, the differences it caused were very small.

D. **References**:

Hsu, F. and A. Oti, "Smoke Chemistry of Reduced Density Rod Cigarettes," memo to R. Kinser, March 8, 1989.

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II. ANALYSIS OF CARBON/IRON SAMPLES BY MOSSBAUER AND LASER MICROPROBE MASS SPECTROMETRY

A. **Objective**: To evaluate the spectra obtained from the laser microprobe mass spectrometry (LAMMA) analysis.

B. **Results**: The LAMMA spectra were obtained at low and high laser energy to identify elemental and molecular composition, respectively. The microscopic differences in elemental composition of a sample were measured at a spatial resolution of approximately 5 um.

C. **Conclusions**: The LAMMA analysis was more useful in characterizing the elemental composition than the molecular composition. The capability of LAMMA to probe the microscopic differences in a sample complements the structural information obtained by Mossbauer spectroscopy and x-ray diffraction spectroscopy. A possible matrix effect prevented a more detailed interpretation of most of the spectra.

D. **Plans**: Group discussion of LAMMA results.

E. **References**:

Shafer K., "Analysis of Heat Source Materials by Laser Microprobe Mass Spectrometry," memo to C. Lilly, April 11, 1989.

III. ANALYSIS OF OXYGEN IN ART SAMPLES

A. **Objective**: To determine the partition coefficient of oxygen in the aqueous and gaseous phase of ART pilot plant drain water under different experimental conditions.

B. **Results**: Instrumentation was set up for the electrochemical detection of oxygen. Oxygen concentrations were measured in the aqueous and gaseous phase after bubbling air and carbon dioxide through the water, respectively.

C. **Conclusions**: Electrochemical detection of oxygen in both phases is possible using the Clark electrode.

D. **Plans**: The electrochemical approach will continue.

E. **References**:

1. Howell, T., "Oxygen Solubility in Pure Water Versus ART Pilot Plant Drain Water Containing Tobacco Solubles," memo to E. B. Fischer, April 4,1989.

2. Shafer, K., PM Notebook #8789, p. 9.

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IV. THERMOGRAVIMETRIC ANALYSIS OF GLUCOVANILLIN AND PROPENYL GUAETHOL GLUCOSIDE

A. **Objective**: The objective of this experiment was to find similarities in the thermal decomposition characteristics of the two compounds for the feasibility of substituting glucovanillin for propenyl guaethol glucoside.

B. **Results**: The samples were analyzed in both TGA and DSC in nitrogen atmosphere with a flow rate of 5°C/min. The two compounds showed similar decomposition patterns both showing evidence of a two step decomposition which is probably the cleavage of the compounds to form vanillin. The only major difference between the two compounds is the amount of residue left after the runs were completed. The residues of the pyrolytic decomposition of propenyl gueathol glucoside and glucovanillin were 1.0 and 10.8 percent, respectively.

C. **Conclusions**: The TGA and DSC showed similar decomposition patterns. Further studies should be done by evolved gas analysis to investigate the decomposition products.

D. **References**:

Chung, C., "Thermal Analysis of Propenyl Guaethol Glucoside and Glucovanillin," memo to J. Chan, March 22, 1989.

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